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Los Alamos, New Mexico 87545

PREDICTION METHODOLOGY FOR CONTAMINANT TRANSPORT FROM RANGELAND WATERSHEDS

M. A. Devaurs*, E. P. Springer*, L. J. Lane*, G. J. Langhorst*
Member ASAE

Weather on arid and semiarid lands can be extremely variable. Runoff is generally emphemeral, and high intensity, short-duration rainfall events are the major stimulus for runoff events. Transport of sediment and associated contaminants occurs with these infrequent events. Incorporation of variability in weather into any prediction technology is essential to provide accurate representations of climate-induced uncertainty in predictions of hydrologic response.

The objective of this study is to investigate a method for including short-term climatic variations in analyses for contaminant transport from rangeland watersheds in arid/semiarid regions. Short term is defined here as a twenty to fifty year time frame and it is assumed that long term climatic fluctuations are not observed during this time. Also, most weather records are available for this time period; predictions of greater length are extrapolations of existing records unless corroborative data for longer term trends are collected.

Predictions are being made with considerable uncertainty in the weather inputs even if the models for water, sediment, and contaminant transport are perfectly known. This study will incorporate uncertainty in weather inputs into the prediction process and address the ramifications of this uncertainty. Uncertainty introduced by improper model or parameter specification is only briefly addressed.

BACKGROUND

Modeling of natural systems has followed two general courses: deterministic and stochastic. In the deterministic approach, a single answer is given for specified parameter set, boundary and initial conditions, and input terms. Stochastic modeling provides a statistical description of the answer so that inferences can be made about various outcomes.

A basic ordinary differential equation describing the water balance per unit area at a site can be written

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$$\frac{ds}{dt} = P - Q - L - ET \tag{1}$$

where s is soil moisture storage; P is precipitation; Q is net runoff; L is deep percolation; and ET is evapotranspiration. The variables in Eq. 1 are in units of volume per unit area per unit time ($L^3/L^2/T$ or L/T). This same equation can be used to describe a deterministic or stochastic system. By making P a random variable, the equation becomes a random ordinary differential equation. S is then a random variable whose distribution depends on P. More formally, Equation 1 can be rewritten as (Soong 1973)

$$\mathring{x}(t) = f[x(t), a(x,t), I(\lambda,t)] \tag{2}$$

$$x(o) = X_0$$

where $\mathring{x}(t)$ is the derivative of X with respect to time; $x(t)$ is the system state variable; $a(x,t)$ is the parameter term; $I(x,t)$ is the input term; and X_0 is the initial value of X. Equation 2 was written in terms of scalars, but it can also be written as a system of equations with each of the terms vectors. If the parameters, initial conditions and inputs, or any combination of these, are random variables, then Equation 2 is a random differential equation, and it must be solved using techniques derived for this class of equations (see Soong 1973).

Analytical solutions to random differential equations are possible if certain conditions are met, but as with deterministic differential equations the assumptions required to obtain analytical solutions limits the class to a very small part of the total domain of interest. A second approach to the solution of random differential equations is to use Monte Carlo methods. Monte Carlo techniques involve sampling the desired variables from a probability distribution and simulating over a specified time period. Generally several simulations are conducted and the state variable(s) are treated independently for each simulation. Either Monte Carlo or analytical results can be presented as either a probability density function (pdf) or moments, of which the mean and variance are the two most popular. A pdf has the advantage of allowing probability statements to be made about the occurrence of certain events.

Monte Carlo techniques have been used by Tiwari and Hobbie (1976) to model aquatic ecosystems and by Arkin et al. (1980) for sorghum production. As discussed earlier, when making predictions of the behavior of natural ecosystems with a stochastic forcing function such as weather, it is prudent to incorporate uncertainty into the analysis to aid in the decision making process.

METHODS

Hydrologic Models

CREAMS: CREAMS (Chemicals, Runoff, Erosion from Agricultural Management Systems) (Knisel 1980) is a field-scale model with hydrology, erosion and sediment components that is to be applied to an area of homogeneous soils.

CREAMS operates on a daily time step, and it requires daily precipitation, maximum and minimum temperatures, and solar radiation. The daily hydrology option (Smith and Williams 1980) uses a modified Soil Conservation Service (SCS) curve number (CN) method to partition precipitation into runoff and infiltration. A soil profile is simulated over the rooting depth and is divided into seven layers.

Evapotranspiration (ET) is calculated using the method from Ritchie (1972). Leaf area index (LAI) is used to partition potential ET into soil evaporation and plant transpiration. Downward movement of soil water occurs when the water content for a layer is greater than field capacity.

Peakflow rates are a critical response variable for the analyses in this study, and in the daily hydrology option of CREAMS, the peakflow is calculated by a modified-rational formula that uses drainage area, watershed length to width ratio, and channel slope.

Contaminant transport predictions require soil erosion rates by sediment particle size classes because of the preferential affinity of most contaminants for smaller particle sizes. The erosion component of CREAMS has been described by Foster et al. (1980). Inputs obtained from the hydrology component include rainfall amount, rainfall erosivity, runoff volume, and peakflow rate. Elements used to simulate fields are overland flow, channel flow, and ponds. Sediment load is assumed to be quasi steady. Equations for detachment on overland flow elements for both interrill and rill erosion are derived from Foster et al. (1977) and they combine the parameters from the Universal Soil Loss Equation (USLE) (Wischmeier and Smith 1978) with rainfall and runoff values. Channel elements use the spatially varied flow equation and a critical shear stress to determine detachment. Both the overland and channel elements use the Yalin equation for sediment transport capacity. Particle size data can be entered into this component to calculate differential sediment load.

ARDBSN: ARDBSN is a watershed-scale model derived from the CREAMS model with components from SWRRB (Simulator for Water Resources on Rural Basins) (Williams et al. 1985). ARDBSN is distributed for both input parameters and rainfall. A scheme for estimating transmission losses (Lane 1982a) has been incorporated into ARDBSN for determining this component in arid/semiarid watersheds.

ARDBSN discretizes a watershed into upland areas or fields, channels, and ponds. Water balance on fields is calculated using the same routines as CREAMS except the soil profile can extend below the rooting depth. Also, subsurface return flow is calculated for the bottom layer in the profile when water content of this layer is greater than field capacity. Peakflow is determined with a modified Rational formula (Lane 1982a) wherein parameters are based on geomorphic characteristics of the watershed (Murphy et al. 1977). Upland sediment yield is estimated by the modified USLE (Williams 1975). No provisions for routing by particle size are included in this model.

Routing of water in channel elements uses a double-triangle hydrograph approximation to distribute flow, and Manning's equation for a rectangular channel to determine sediment transport capacity. Typically channels found in arid/semiarid watersheds have alluvial bottoms, so sediment yield is for the most part transport limiting. Using the transport capacity, the channel sediment yield is calculated by particle size class (Lane 1982b).

Weather Generator

The program WGEN (Richardson and Wright 1984) was used to generate the daily sequences of maximum and minimum temperatures, precipitation, and solar radiation. WGEN is designed to maintain temporal dependence, cross correlations, and seasonal characteristics of weather data at a location. The temperatures and solar radiation are generated with autocorrelation and cross correlations preserved and whether it is a dry or wet day. Seasonal variations in the mean and coefficient of variation of the maximum and minimum temperatures and solar radiation are described by a cosine series.

Daily precipitation is generated by a Markov Chain that describes the sequence of wet and dry days and a two-parameter gamma probability density function determines the daily precipitation amount on a wet day.

Study Locations

Walnut Gulch: The Walnut Gulch Experimental Watershed has been operated by the United States Department of Agriculture, Agricultural Research Service (USDA-ARS) since 1962 (Renard 1970). The watershed is located southeast of Tucson, Arizona and the city of Tombstone is located in the 149 km^2 watershed (Fig. 1).

In this study, two subwatersheds of the Lucky Hills watershed complex were used. Watersheds 63.101 and 63.103 have areas of 0.01 and 0.04 km^2, respectively. A seventeen year precipitation, sediment yield and streamflow record from both of these watersheds was used in subsequent analyses (Table 1).

Table 1. Seventeen year peakflow discharge records for Lucky Hills Watersheds 1 and 3 located in the Walnut Gulch Experimental Watershed, Arizona.

Year	Watershed 1 Qp (m^3/s)	Watershed 3 Qp (m^3/s)
1965	0.26	0.48
1966	0.13	0.10
1967	0.12	0.16
1968	0.12	0.27
1969	0.06	0.11
1970	0.24	0.48
1971	0.28	0.53
1972	0.11	0.21
1973	0.20	0.47
1974	0.10	0.21
1975	0.42	0.87
1976	0.16	0.42
1977	0.16	0.35
1978	0.13	0.17
1979	0.06	0.12
1980	0.07	0.10
1981	0.14	0.16
$\bar{X}$	0.16	0.31
s	0.09	0.21

Plutonium Valley: The Plutonium Valley watershed is located on the Nevada Test Site (NTS) in southern Nevada (Fig. 1). This 33 km^2 watershed is part of the closed desert basin that drains into Yucca Lake. The region is arid with average annual precipitation of 15.2 cm (6 in.) for the seventeen years of record from the Yucca Lake weather station. In the late 1950s, Plutonium Valley was the site for safety shots in which a chemical explosive was detonated to determine the possibility of atomic weapons going critical on impact. The purpose of this study is to develop a technique to predict plutonium transport from the watershed.

There are no streamflow or sediment yield records from Plutonium Valley. Various cooperators (see Simanton et al. 1986) conducted rainfall simulator experiments during the spring and fall for the period 1983-1985. These data were used for estimating parameter values for the hydrologic modeling discussed in the following sections.

Procedure

Contaminant transport by surface runoff is a function of contaminant amounts in solution and adsorbed to sediment particles. Therefore, prediction of transported material depends on accurate prediction of water and sediment. In arid and semiarid watersheds, it is the large events, annual peaks and greater, that are responsible for most of the sediment yield, and hence contaminant, movement. Rather than attempt to predict daily hydrographs for the watersheds, the annual flood frequency curve was used to assess our capability to predict hydrologic response.

As previously noted, the Plutonium Valley Watershed has an inadequate streamflow record so Walnut Gulch Watershed data were used to test predictive capabilities of the models. To incorporate uncertainty in the weather data, fifty sequences of seventeen years were generated and used in the hydrologic simulations. The fifty flood frequency curves generated by the simulation procedure were compared to the single observed flood frequency curve. Plotting positions for the flood frequency curves were determined by the Weibull method (Haan 1977) which is

$$\frac{m}{(n + 1)}$$

where m is the rank of a given event in ascending order; and n is the total number of events.

A similar procedure was followed for the contaminant transport simulations at Plutonium Valley, but no observed data were available for comparison. In this case, cumulative transport by plutonium over the seventeen year period was the variable plotted on probability paper.

RESULTS AND DISCUSSION

Flood Frequency

Initial simulations with CREAMS on Lucky Hills 1 (LH1) and Lucky Hills 3 (LH3) revealed that the observed flood frequency curve was greater than the mean plus one standard deviation curve for the fifty simulations (Figs. 2 and 3). Parameter values for CREAMS were determined using handbook values and knowledge of Walnut Gulch which would lead to the conclusion that parameter values were inadequate. To ascertain if parameter values were the problem, CREAMS was calibrated using the observed precipitation and peakflow records, and simulations with the fifty generated sequences were repeated. These data are presented in Figs. 4 and 5. The observed values appear to approach the mean plus one standard deviation curve, but do not fall within this range. To make predictions, it is desirable to avoid procedures such as model calibration because data are not generally available for these purposes. However, even with calibrated data, the observed curve does not fall into the desired range. In terms of predicting contaminant transport, values would be underestimated if these sequences were used in making predictions.

Sources of Error

First, it must be acknowledged that only a single 17 year sequence of data from each watershed is being used for comparison. A probability exists that the observed data do have the relationship with the generated data presented in Figs. 2-5. This is a dilemma when limited data are available. For this study, it has been assumed that the observed data do represent average conditions expected on these watersheds for the time horizon of concern. Longer term predictions, 50 to 100 years, will be extrapolating the data and the observed data may not be representative of conditions over the extended time frame. For this purpose, we simulated only for the length of record available.

Two possible sources of error were investigated: model formulation and stochastically generated precipitation input. The possibility that CREAMS is an inadequate model for the given system was tested using ARDBSN. This does not represent a complete evaluation because many of the same processes that govern the distribution of water in CREAMS are found in ARDBSN. Channel components including channel losses are in ARDBSN and not CREAMS.

Initial parameter values to apply ARDBSN to LH3 were found in Renard et al. (1983, 1987) for the entire Lucky Hills Watershed. Using these parameter values, the observed flood frequency was consistently greater than the simulated mean plus one standard deviation. The model was calibrated and the simulations were repeated with the same result (Fig. 6).

Consistent underprediction by both models led to testing the values being produced by the weather generator, WGEN. How did the maximum daily precipitation values generated by WGEN compare to the 17 year observed record?

Figure 7 is a histogram of the frequency of occurrence of the maximum annual daily precipitation compared to the same variable extracted from 50 simulations of 17 years by WGEN. One possibility is that generated values may not be following the seasonal distribution and this may affect the annual peakflow value through antecedent moisture conditions. However in Fig. 7 there do not appear to be any major discrepancies between the distribution of generated and observed values.

The next variable to be examined was the magnitude of the generated annual maximum daily precipitation values (Fig. 8). In Fig. 8, the maximum daily value for each 17-year realization from the 50 generated sequences is plotted with the observed 17 year maximum annual values. Seasonal distributions are obtained by plotting these values in the month in which they occurred. As in Fig. 7, the seasonal distribution of observed and generated values appears to correspond quite well. However, it is immediately evident that two observed values exist whose magnitude is not obtained in the generated sequences (Fig. 8). Recall that the generated values in Fig. 8 are the maximum daily precipitation value for 17 years, so all other maximum daily values are less than the plotted values.

These data are indicative of the potential problem in using a weather generator to simulate weather patterns in arid and semiarid ecosystems where infrequent large events are dominant. It appears that the tail of the gamma pdf is not sampled sufficiently, resulting in peakflow rates biased towards lower values. WGEN reproduces the mean, variance, and temporal distribution of precipitation well, but extreme values do not appear to be sampled.

A constraint placed by Richardson and Wright (1984) on WGEN was that the shape parameter for the gamma distribution be less than 1. The scale parameter was determined from the value of the shape parameter (Haan 1977). Using the same maximum likelihood estimation (MLE) procedure as Richardson and Wright (1984), new values for the parameters were calculated (Table 2). The WGEN computer code was then modified to

Table 2. Gamma probability density function parameters for Lucky Hills simulations using WGEN before and after constraint of shape parameter, B, being less than 1 is removed.

	Before		After	
Month	α	B	α	B
JAN	0.192	0.998	0.160	1.195
FEB	0.211	0.998	0.190	1.111
MAR	0.205	0.998	0.139	1.467
APR	0.102	0.998	0.065	1.566
MAY	0.142	0.998	0.135	1.051
JUN	0.192	0.998	0.156	1.226
JUL	0.279	0.991	0.279	0.991
AUG	0.283	0.906	0.283	0.906
SEP	0.302	0.964	0.302	0.964
OCT	0.291	0.930	0.291	0.930
NOV	0.167	0.998	0.104	1.610
DEC	0.209	0.998	0.191	1.094

generate precipitation amounts when the shape parameter is greater than 1 using the procedure in Haan (1977). Results in terms of the flood frequency curve for Lucky Hills Watershed 3 using CREAMS are presented in Fig. 9. There is no improvement in the estimated flood frequency value and upon examining Table 2, the reason is quite apparent. During the months when the peakflows are most likely generated, July and August, there was no change in gamma pdf parameters. Therefore, a higher magnitude would not be generated for the given sequence of random numbers.

Neither errors in the models or the precipitation generation routine are eliminated as possible sources of error. The ARDESN model in particular was designed to simulate the hydrologic response of arid and semiarid watersheds. Even calibrating both hydrologic models to the observed peakflow and runoff volume did not improve simulation results. Both models were calibrated to the mean and variance of the observed peakflow and runoff volume. Perhaps, another statistic should have been selected for the objective function.

The relatively low precipitation magnitude has been discussed. In arid and semiarid ecosystems, it is the timing and magnitude of the event that determines the hydrologic response. Timing is important because events are generally clustered and initial moisture contents are affected by antecedent precipitation. There did not appear to be any seasonal or timing problems with the generated precipitation, but the clustering was not examined. The magnitude of maximum precipitation events appears low, and further research is needed to determine if this was the critical factor in low flood frequency curve estimates.

Contaminant Transport

Despite the shortcomings noted in the previous section, the proposed methodology to predict contaminant transport is independent of simulation model strengths and weaknesses. In the subsequent discussions it is assumed that the models are validated for the area where predictions are being made.

A 4 ha (10 acre) small watershed in Plutonium Valley was used to demonstrate the proposed methodology. Soils data were obtained from Essington and Romney (1986) and Hunter and Greger (1986) for Plutonium Valley. Rainfall simulator data were analyzed to provide values for runoff and USLE parameters for the erosion component of CREAMS. Three sediment particle size classes were assumed for determining particle size distribution to transport plutonium (Pu). No information was available on the distribution of Pu with soil fractions, so distributions presented by

Essington and Romney (1986) for cesium at Plutonium Valley were used. Parameters used in the hydrology and erosion components of CREAMS are presented in Table 3.

Table 3. Parameters for Plutonium Valley, NV simulations for the CREAMS model for both current and treated conditions.

Parameter	Current Value	Treated Value
Condition II CN	70	90
Slope	0.02	0.02
Length-Width Ratio	2	2
Porosity	0.30	0.30
Fifteen Bar Water Content	0.045	0.045
Clay Fraction	0.007	0.007
Silt Fraction	0.145	0.145
Sand Fraction	0.848	0.848
USLE K Factor	0.043	0.043
USLE C Factor	0.011	0.45

Again fifty realizations, each 20 years long, of weather data were generated using WGEN. These data were used to drive CREAMS. Total sediment yield by particle size class at the end of the twenty year simulation is used with cesium data from Essington and Romney (1986) to predict Pu transport. Results are presented in Fig. 10 for current and treated conditions. The treated condition consisted of removing vegetation, disturbing the surface soil and removing 90 percent of the Pu in the soil. This treatment increased the potential for runoff and erosion (Fig. 11). In fact, the increase was large enough that even with 90 percent of the Pu removed, there was still more Pu transported under the treated condition than under the natural, undisturbed conditions.

SUMMARY AND CONCLUSIONS

A methodology was presented that uses stochastic weather generation in conjunction with hydrologic, erosion, and contaminant transport models to predict contaminant transport. Results are presented statistically to reflect the uncertainty in future weather patterns.

Initial tests of the method revealed that flood frequency curves for two watersheds at Walnut Gulch near Tombstone, AZ were underpredicted. The two hydrologic models tested produced similar results. Comparison of generated annual daily maximum precipitation values with 17 years of observed record found that the two maximum values in the observed record were not attained in the generated record. The inability to represent the flood frequency curve is a major limitation and must be remedied before this procedure is applicable. Further investigation of the statistical properties of generated weather data is needed. Apparently, hydrologic models such as used herein provide a logical tool to use in evaluating weather generators such as WGEN.

The methodology was used to predict contaminant transport on the Plutonium Valley Watershed located on the Nevada Test Site. No comparison to observed data was possible. Parameter values for hydrologic and erosion models were obtained from rainfall simulator experiments conducted at the site. Predictions were made for current conditions and for a remedial action that removed 90 percent of the Pu contaminant but also removed vegetation and disturbed the surface soil. Fifty realizations were generated for each of the two conditions and results presented as probability plots.

ACKNOWLEDGEMENT

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Fig. 1 Location of Walnut Gulch and Plutonium Valley

Fig. 2 Observed peakflow discharge rate plotted against mean ± one standard deviation of fifty simulations for Lucky Hills Watershed 1

Fig. 3 Observed peakflow discharge rate plotted against mean ± one standard deviation of fifty simulations for Lucky Hills Watershed 3

Fig. 4 Observed peakflow discharge rate plotted against mean ± one standard deviation for calibrated parameter values for CREAMS using fifty stochastic weather sequences for Lucky Hills Watershed 1

Fig. 5 Observed peakflow discharge rate plotted against mean ± one standard deviation for calibrated parameter values for CREAMS using fifty stochastic weather sequences for Lucky Hills Watershed 3

Fig. 6 Observed peakflow discharge rate plotted against mean ± one standard deviation for fifty simulations using the ARDBSN model for Lucky Hills Watershed

Fig. 7 Frequency of occurrence of maximum annual daily precipitation compared to same variable extracted from 50 simulations of 17 years by WGEN

Fig. 8 Annual maximum daily precipitation value for each 17-year realization from the 50 generated sequences plotted with the observed 17-year maximum annual values (The following observed values, by Julian date, are not visible on the plot: 200, 2.82; 204, 3.28; 206, 2.79; 208, 3.99; 209, 1.91; 210, 2.08; 211, 2.90; 233, 2.67; 237, 1.96; 250, 2.36)

Fig. 9 Observed peakflow discharge rate plotted against mean ± one standard deviation for fifty simulations from Lucky Hills Watershed 3 using CREAMS

Fig. 10 Probability plot of total contaminant yield at the end of 17 years for Plutonium Valley Watershed using natural or current conditions and bare or treated conditions that assumed 90 percent removal of contaminant

Fig. 11 Probability plot of total sediment yield as predicted by CREAMS at the end of 17 year realization for fifty stochastically generated weather sequences for Plutonium Valley, NV

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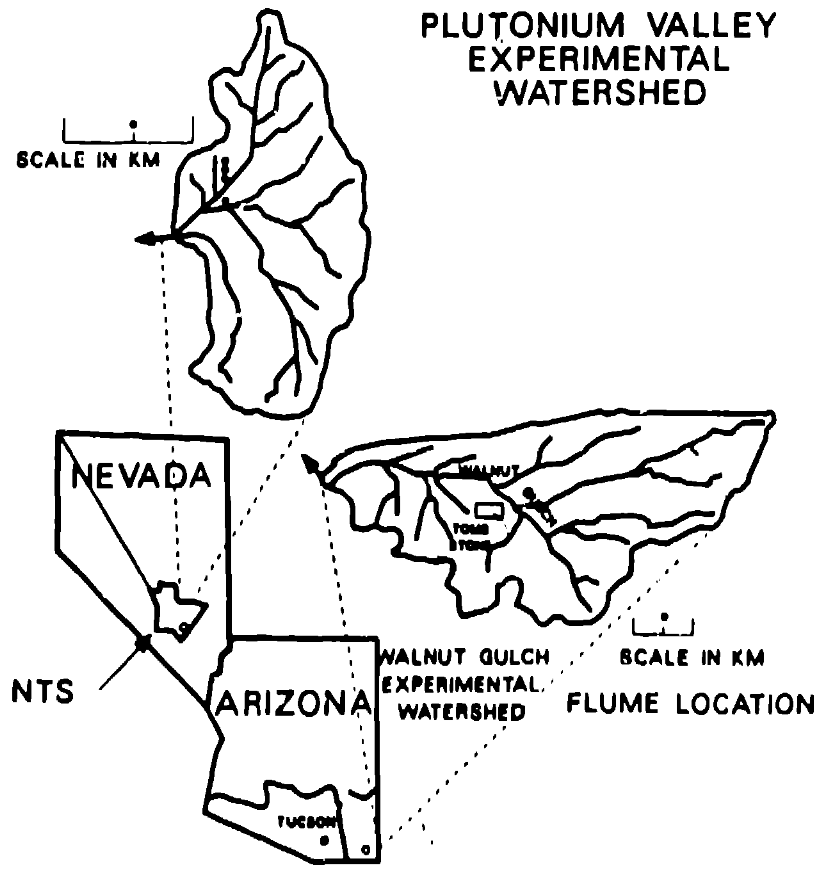


Figure 1

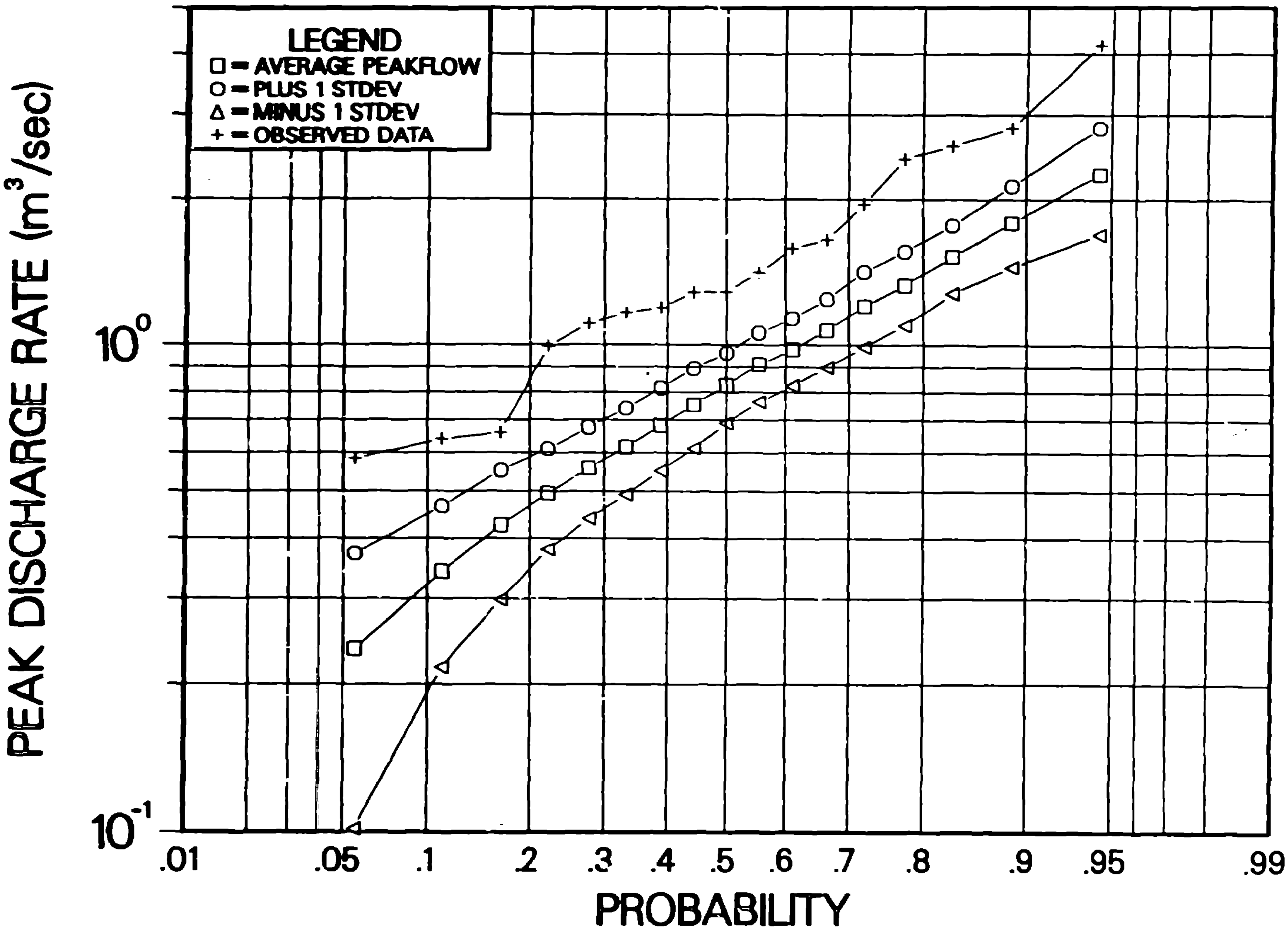

LEGEND
□ = AVERAGE PEAKFLOW
○ = PLUS 1 STDEV
Δ = MINUS 1 STDEV
+ = OBSERVED DATA
PEAK DISCHARGE RATE (m³/sec)
10⁰
10⁻¹
.01
.05
.1
.2
.3
.4
.5
.6
.7
.8
.9
.95
.99
PROBABILITY

Figure 2

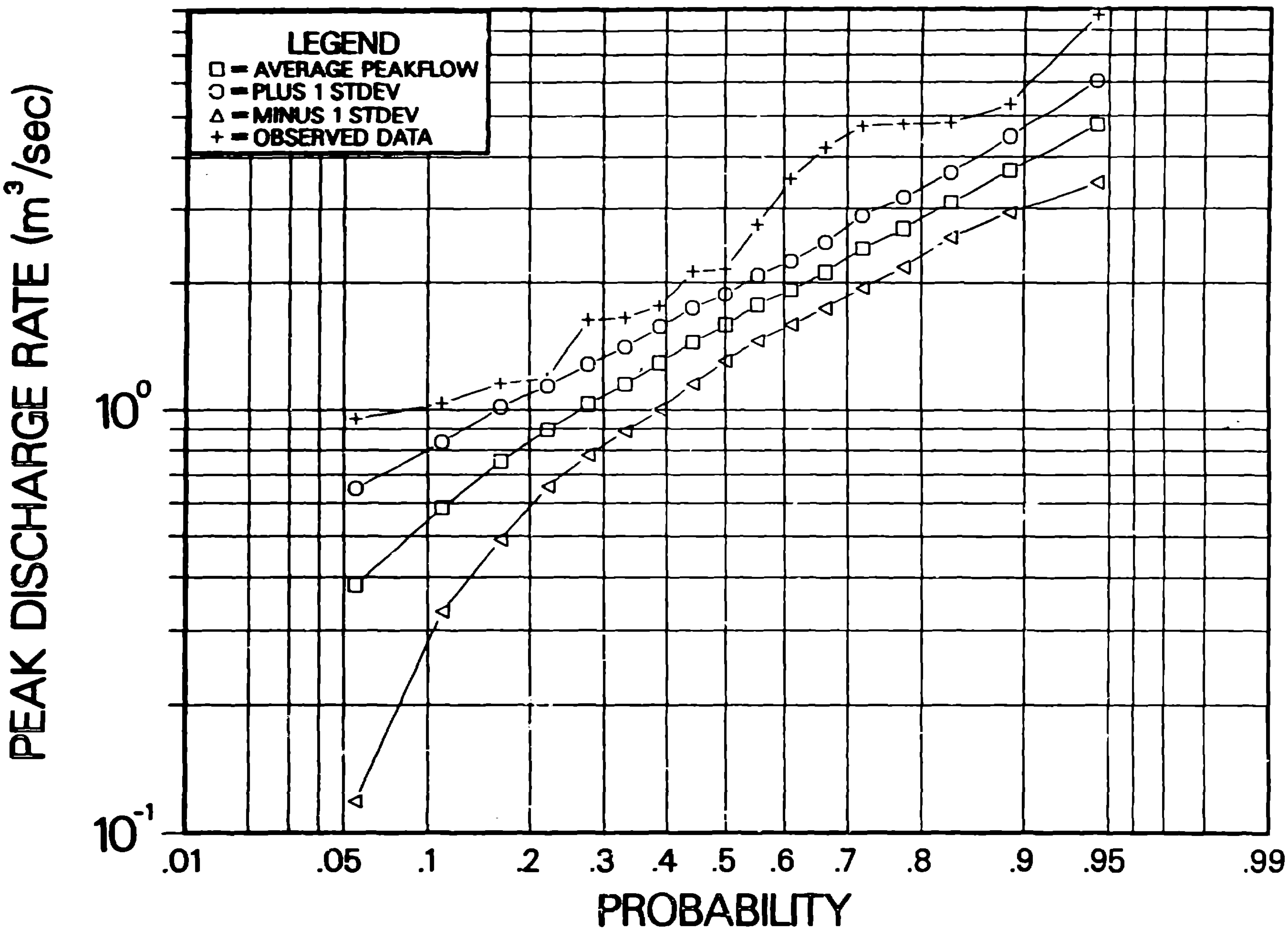

LEGEND
□ = AVERAGE PEAKFLOW
○ = PLUS 1 STDEV
△ = MINUS 1 STDEV
+ = OBSERVED DATA
PEAK DISCHARGE RATE (m³/sec)
10⁰
10⁻¹
.01
.05
.1
.2
.3
.4
.5
.6
.7
.8
.9
.95
.99
PROBABILITY

Figure 3

DRAFT

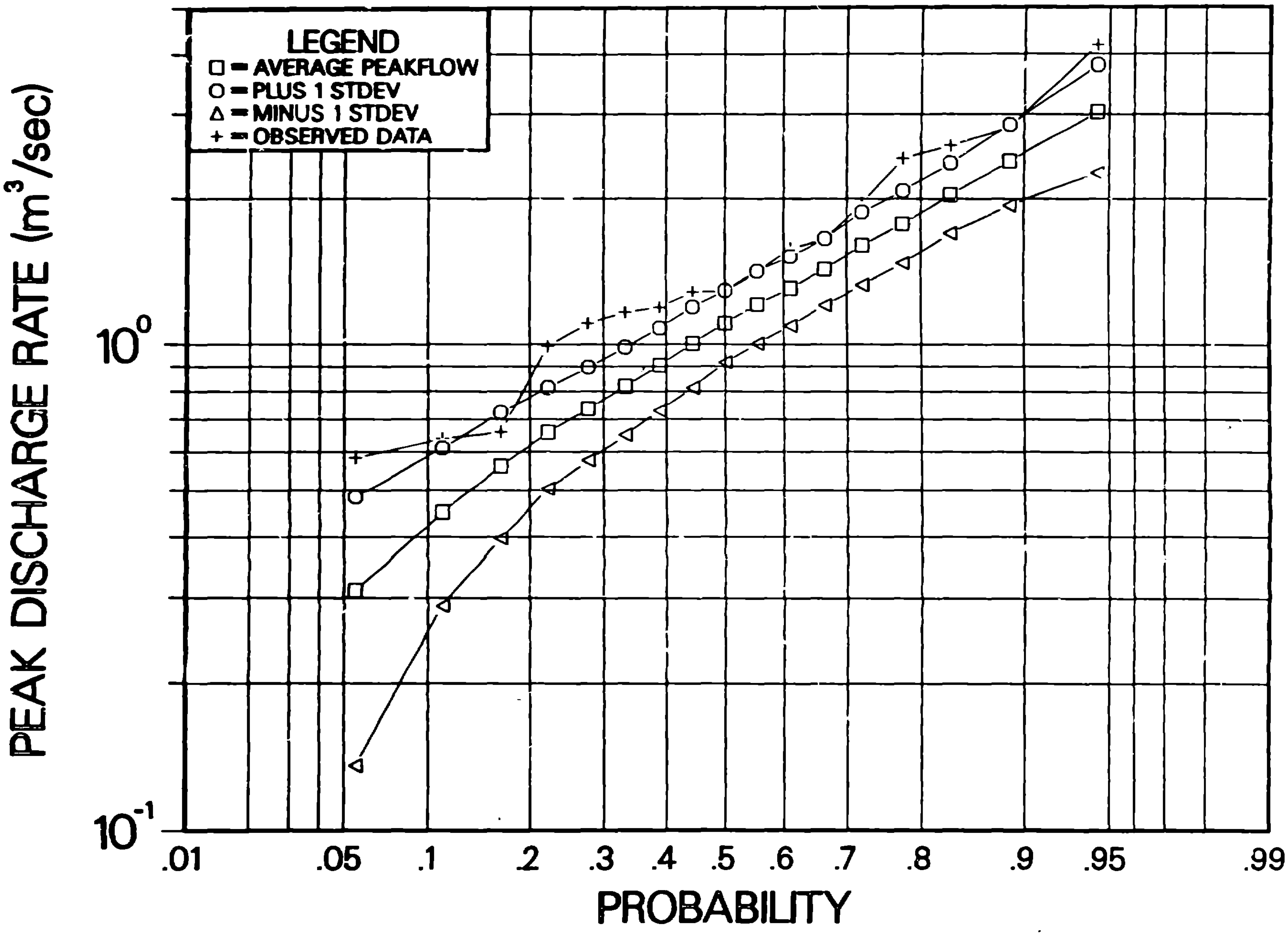


Figure 4

DRAFT

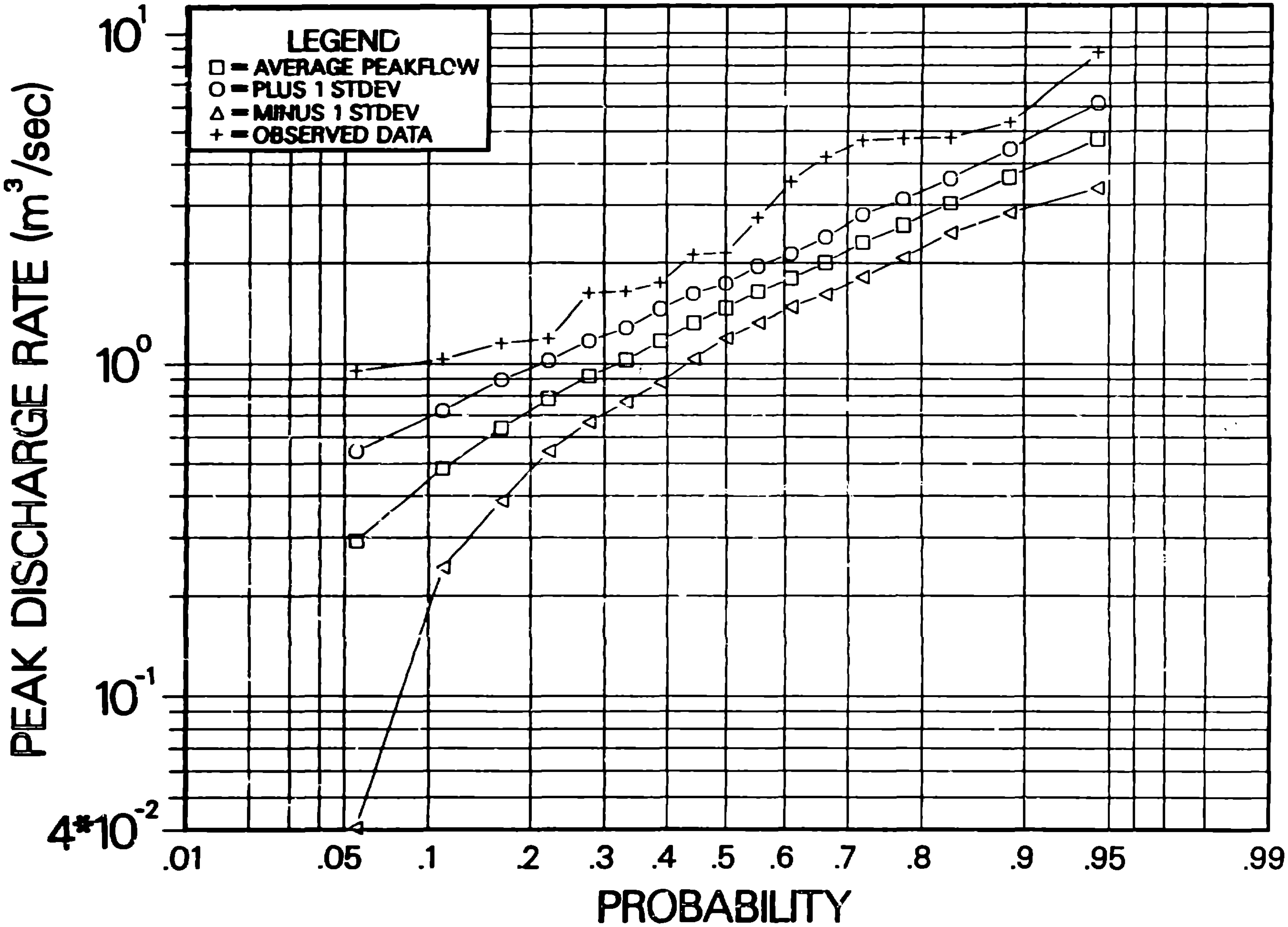


Figure 5

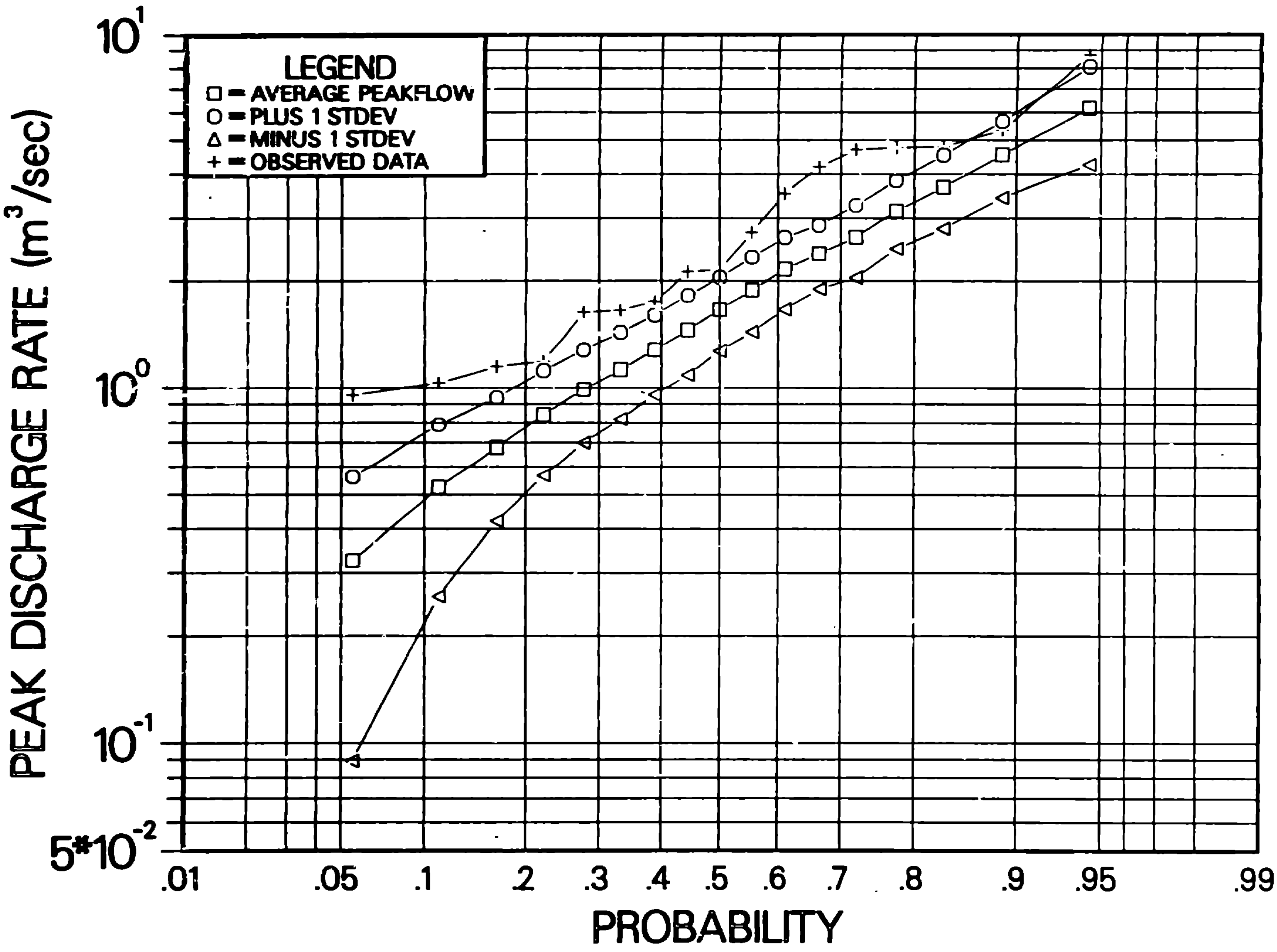
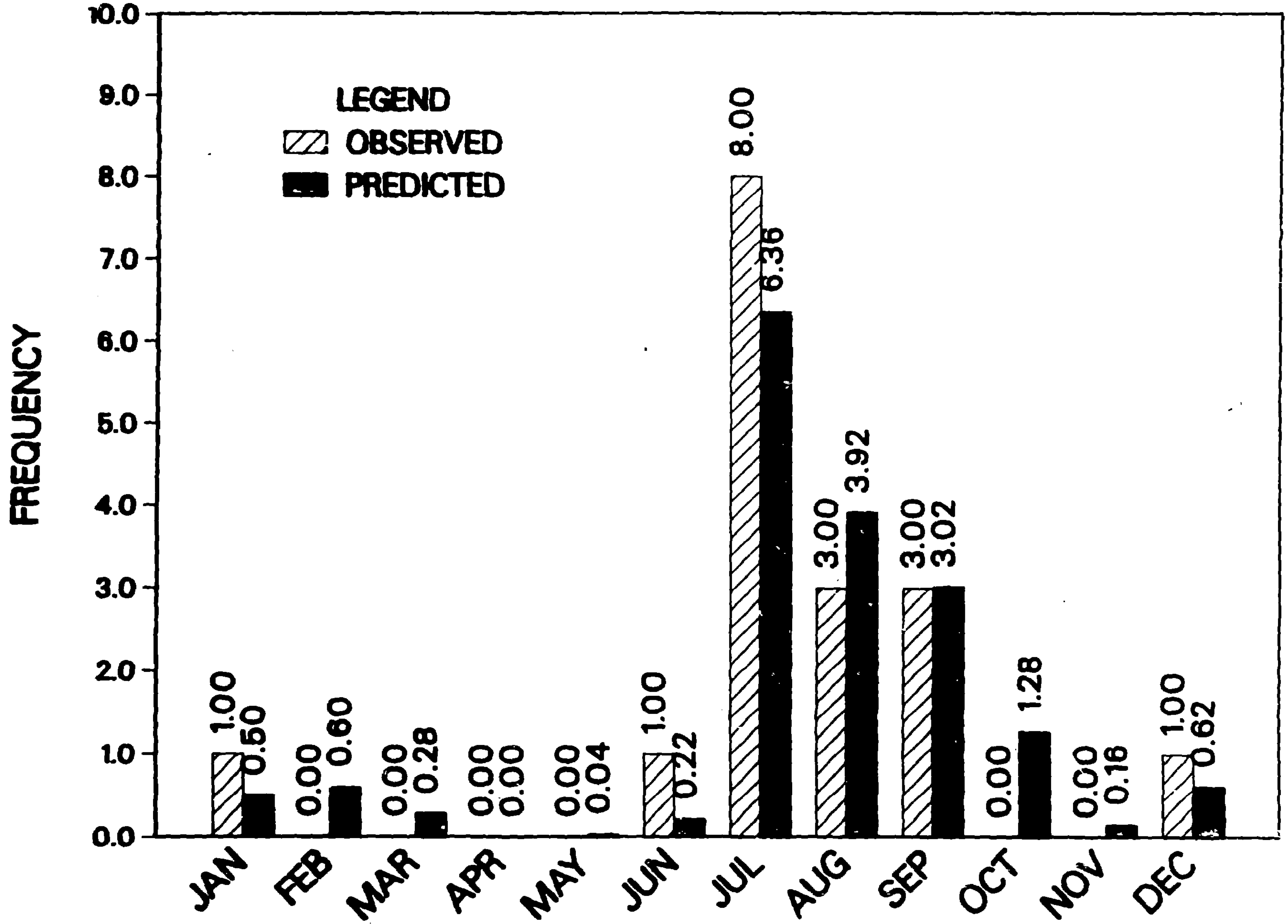

LEGEND
□ = AVERAGE PEAKFLOW
○ = PLUS 1 STDEV
Δ = MINUS 1 STDEV
+ = OBSERVED DATA
PEAK DISCHARGE RATE (m³/sec)
10¹
10⁰
10⁻¹
5*10⁻²
.01
.05
.1
.2
.3
.4
.5
.6
.7
.8
.9
.95
.99
PROBABILITY

Figure 6



LEGEND
OBSERVED
PREDICTED
FREQUENCY
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
1.00
0.50
0.00
0.60
0.00
0.28
0.00
0.00
0.00
0.04
1.00
0.22
8.00
6.36
3.00
3.92
3.00
3.02
0.00
1.28
0.00
0.16
1.00
0.62
JAN
FEB
MAR
APR
MAY
JUN
JUL
AUG
SEP
OCT
NOV
DEC

Figure 7

DRAFT

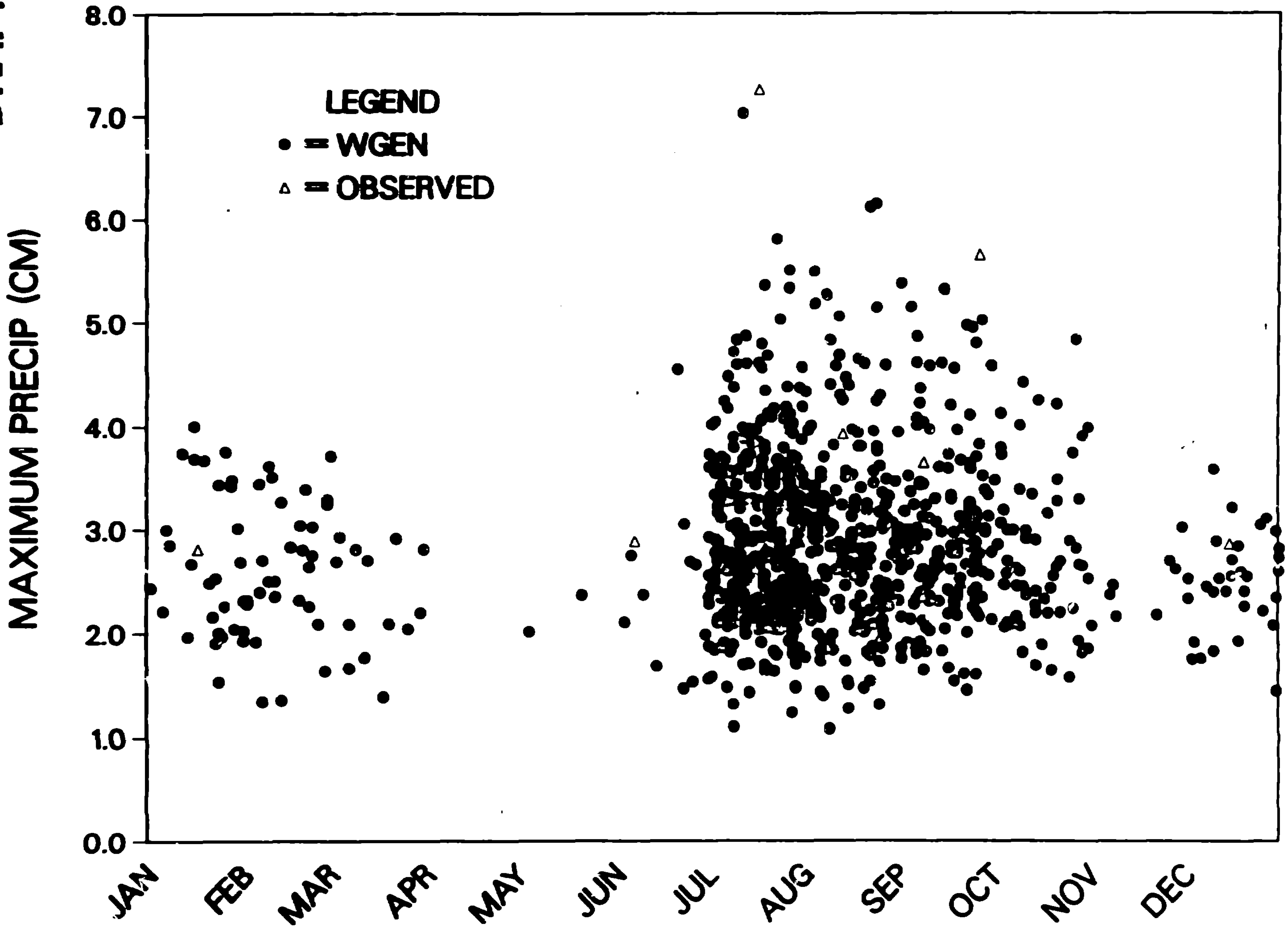


Figure 8

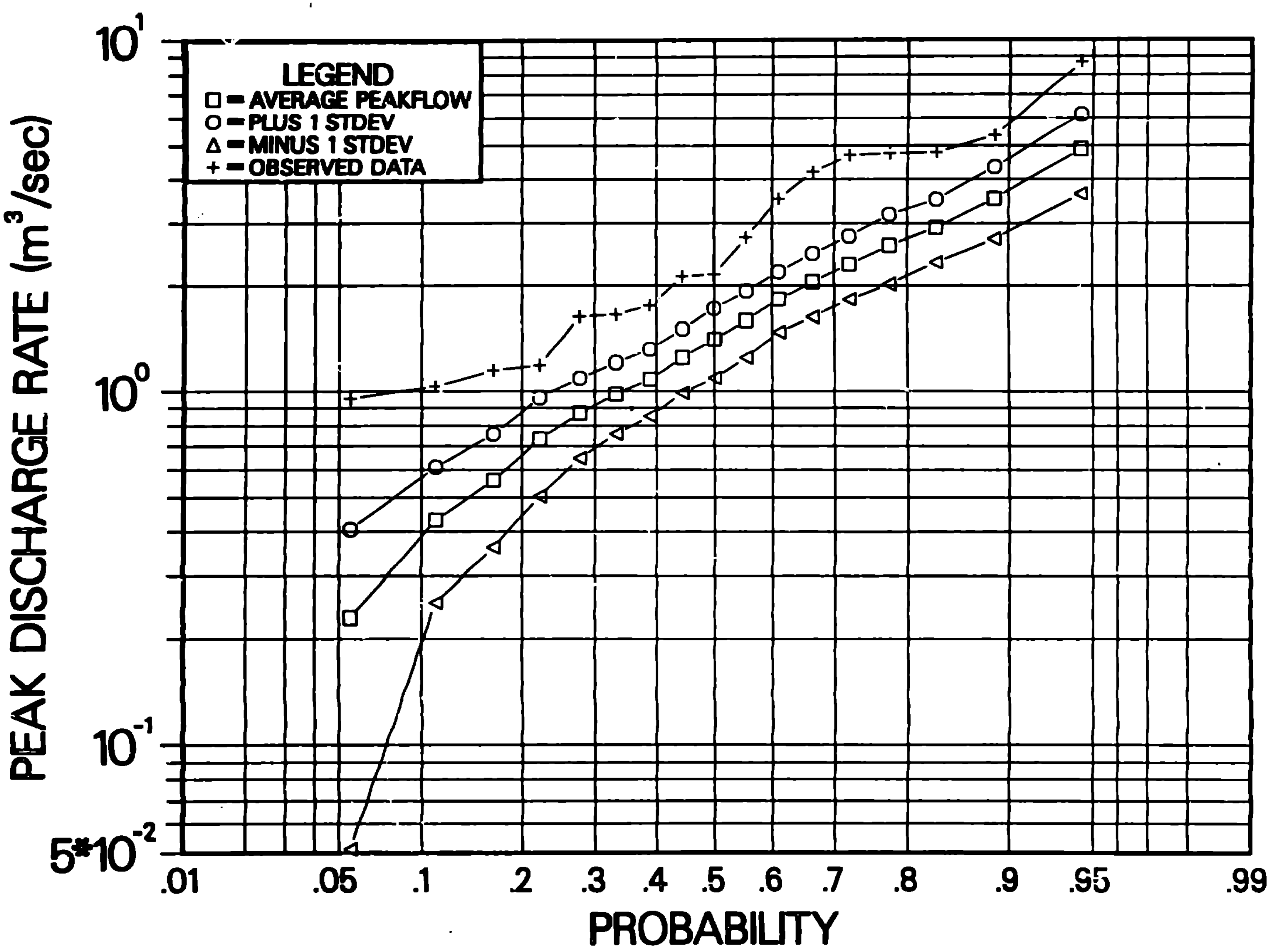

LEGEND
□ = AVERAGE PEAKFLOW
○ = PLUS 1 STDEV
Δ = MINUS 1 STDEV
+ = OBSERVED DATA
PEAK DISCHARGE RATE (m³/sec)
10¹
10⁰
10⁻¹
5*10⁻²
.01
.05
.1
.2
.3
.4
.5
.6
.7
.8
.9
.95
.99
PROBABILITY

Figure 9

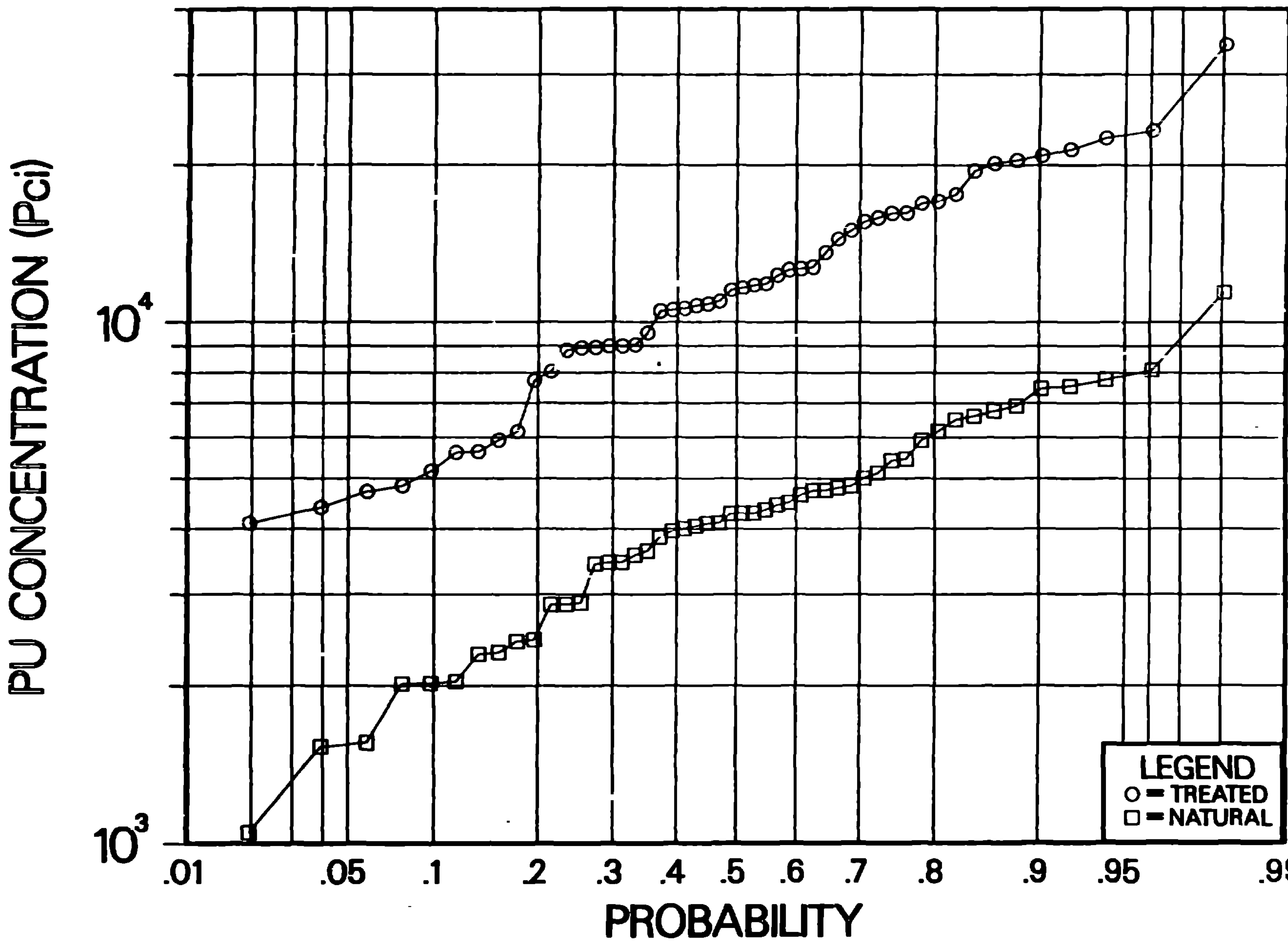

PU CONCENTRATION (Pci)
10^4
10^3
.01
.05
.1
.2
.3
.4
.5
.6
.7
.8
.9
.95
.99
PROBABILITY
LEGEND
○ = TREATED
□ = NATURAL

Figure 10

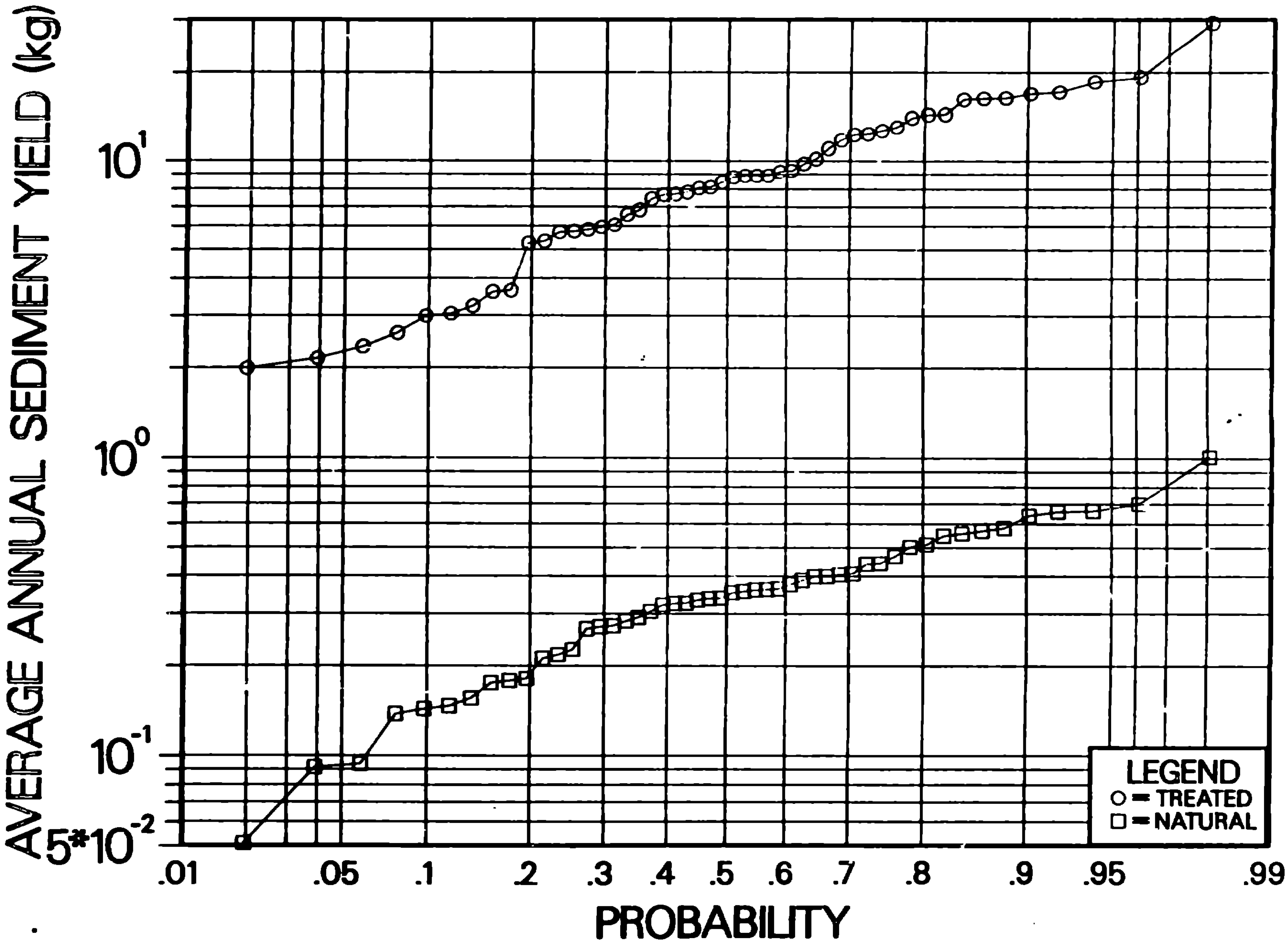

AVERAGE ANNUAL SEDIMENT YIELD (kg)
10^1
10^0
10^-1
5*10^-2
.01
.05
.1
.2
.3
.4
.5
.6
.7
.8
.9
.95
.99
PROBABILITY
LEGEND
○ = TREATED
□ = NATURAL

Figure 11